Applications of quantum transport in devices

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California Institute of Technology

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Application of Quantum Transport in Devices

- **What is the focus of the research?**

  - **Quantum Transport**
    => Devices/Structures are a tool to explore the needed theory
    - Relevant Theories:
      Green Functions, Wigner Functions, Rate Equations
    - Relevant Structures:
      quantum dots/wires, molecules, RTDs (for time dependence only)

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    => Quantum transport is a tool to design/optimize devices
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    - Need quantitative agreement between experiment and theory
      - DC, high bias performance
      - AC / time-dependent high bias performance
    - Need realistically sized devices - contacts/reservoirs.
    - Need realistic electron interactions with environment:
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Quantitative Modeling of Devices

Quick review of DC transport simulations in RTDs - NEMO 1-D

- **Realistic contacts:**
  - **Quantized and continuous states in the emitter**
- **Realistic bandstructure:**
  - **Band-non parabolicity - emitter states and RTD state alignment**
- **Putting it together:**
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  - **Bistability (in symmetric structures) a numerical problem due to limited device models**
  - **Test matrix - comparison to experiment**

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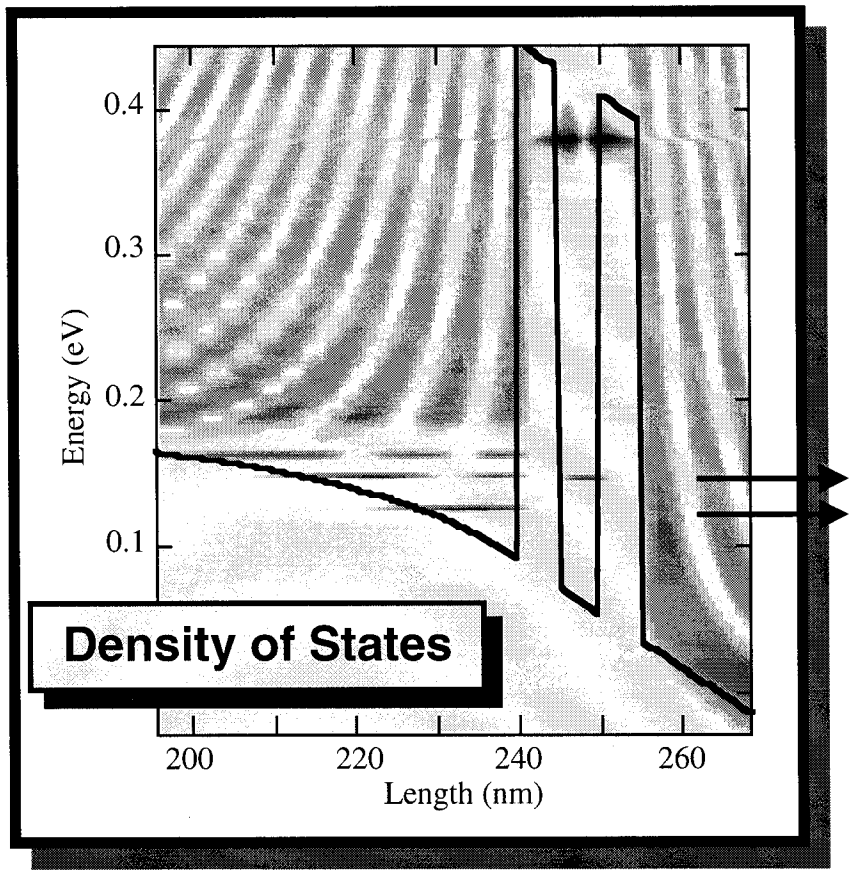

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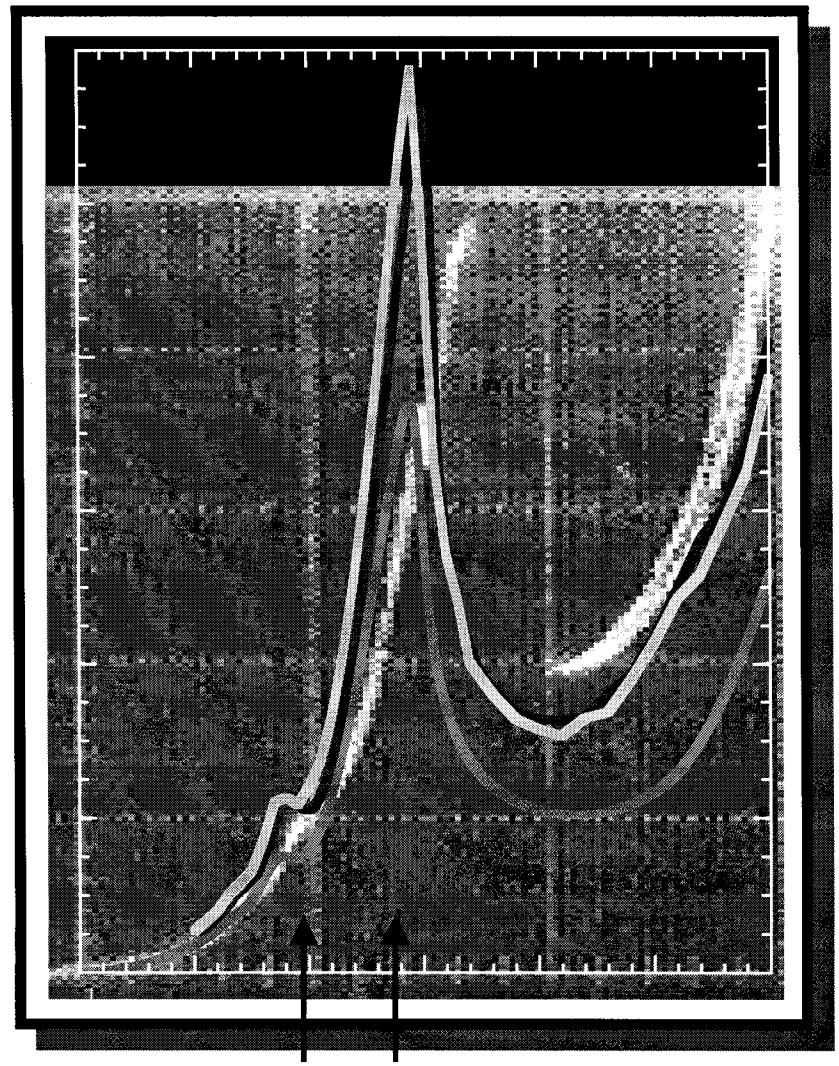

Quantum selfconsistent potential

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Band non-parabolicity modifies momentum dependence in emitter-RTD coupling

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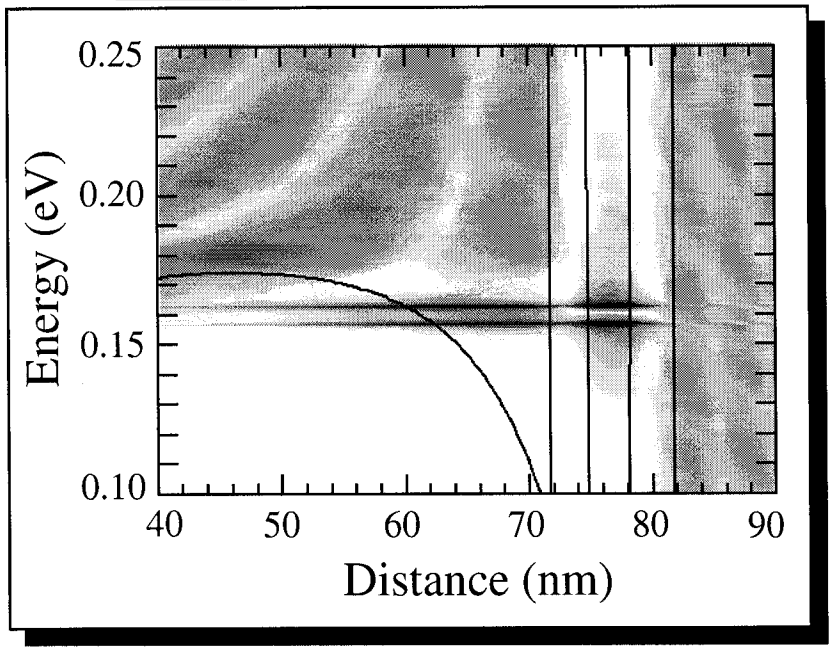

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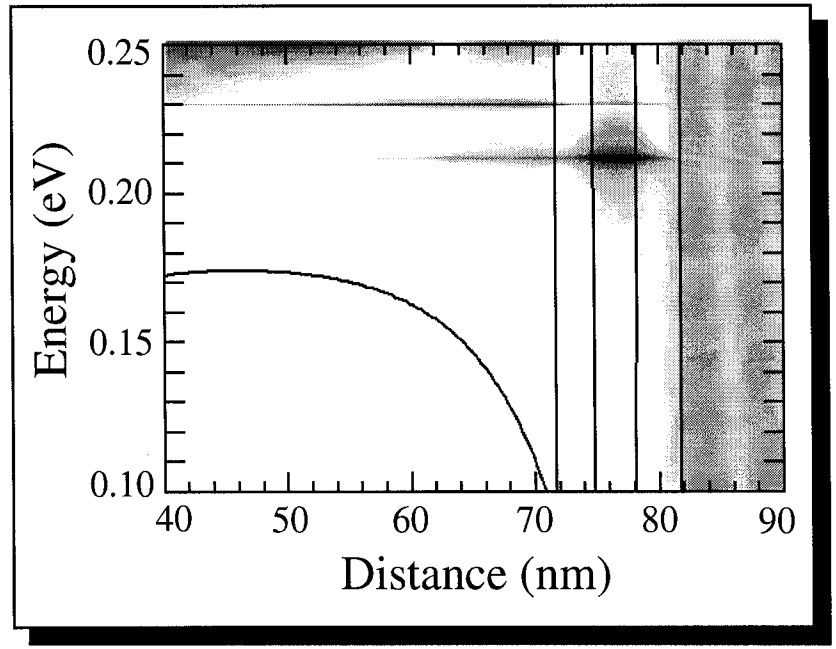

Resonance coupling depends on the transverse momentum

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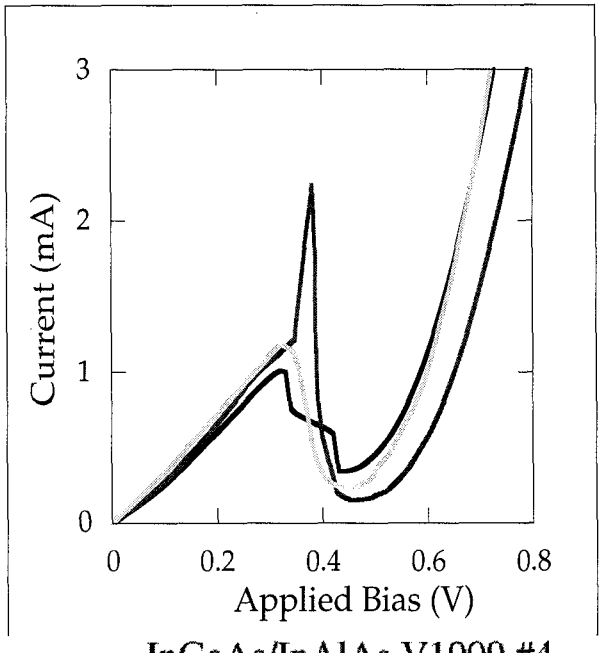

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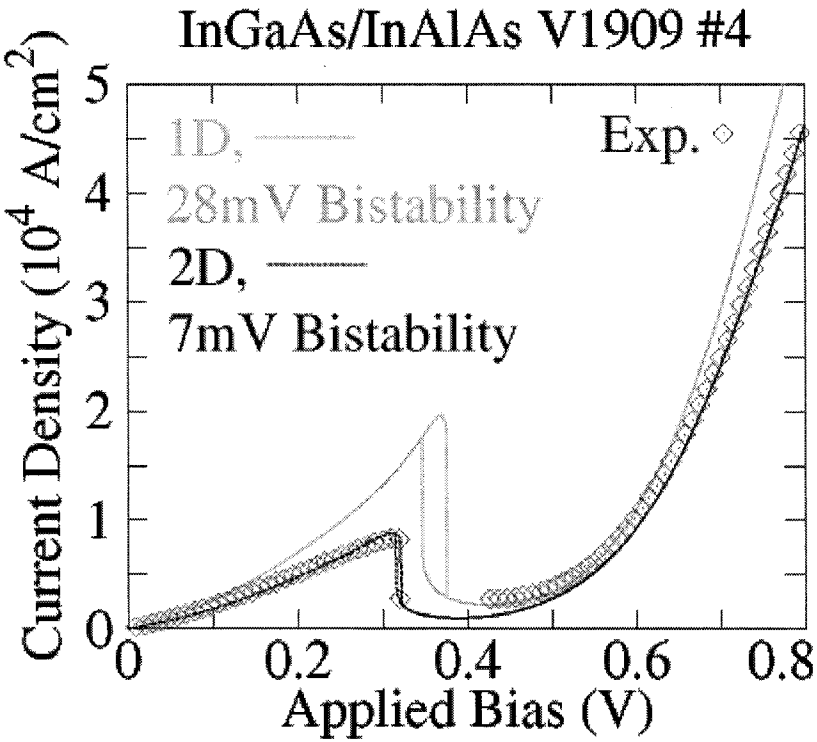
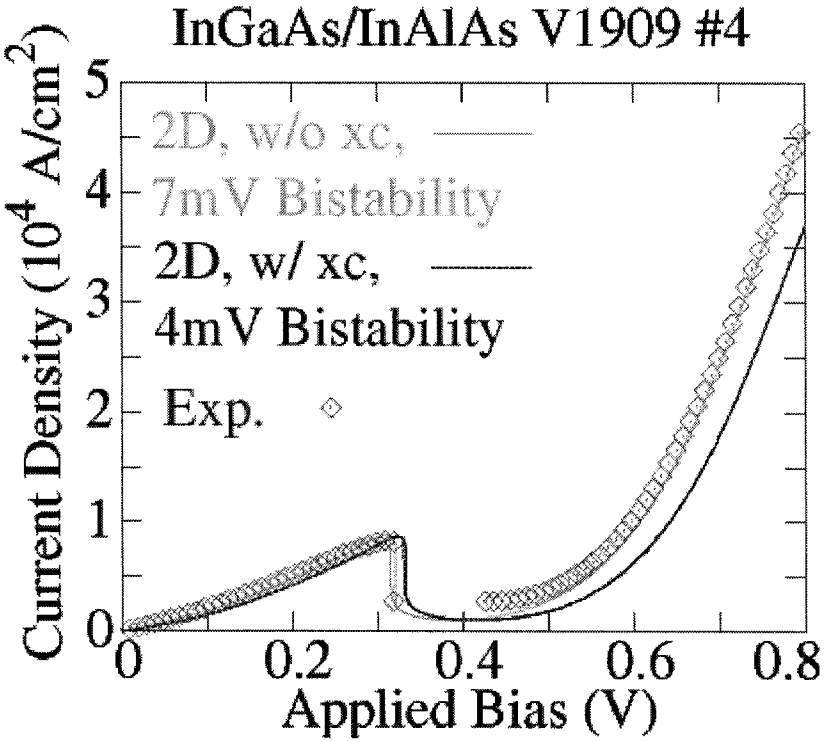
Full band integration + Exchange&Correlation





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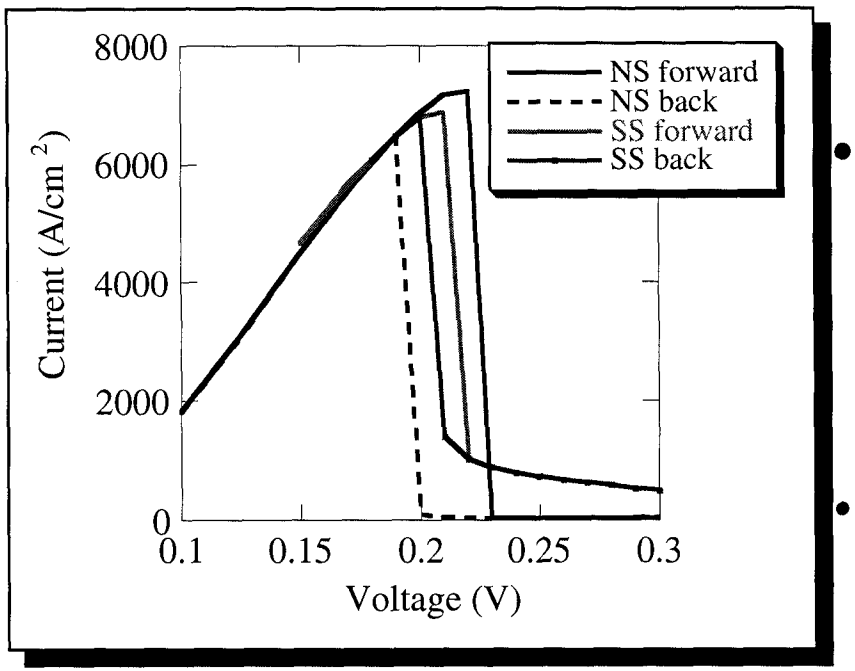

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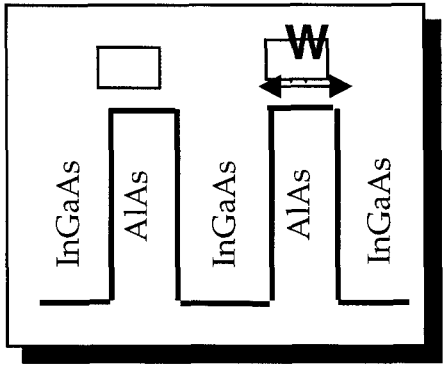

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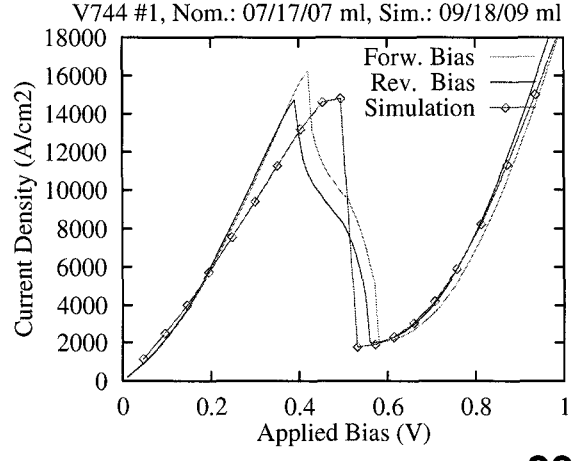

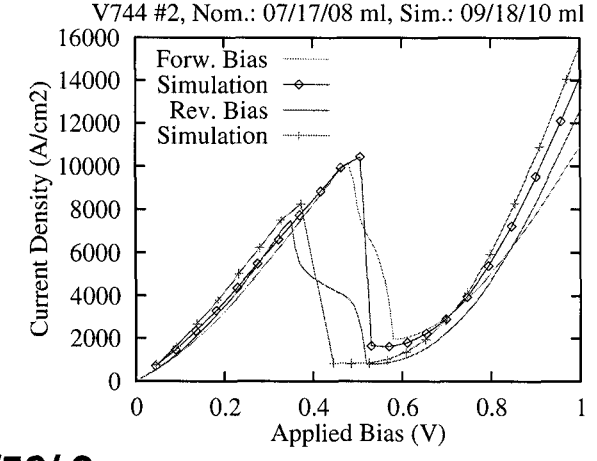

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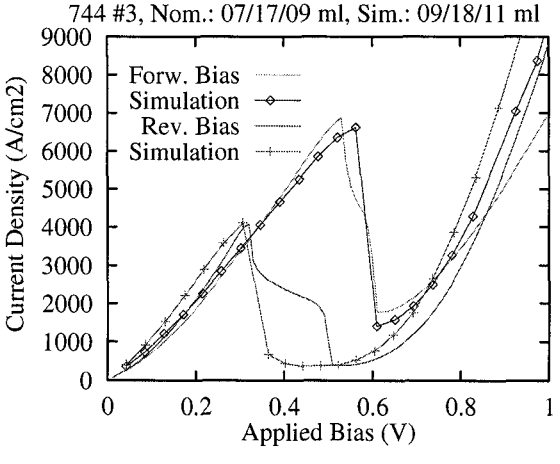

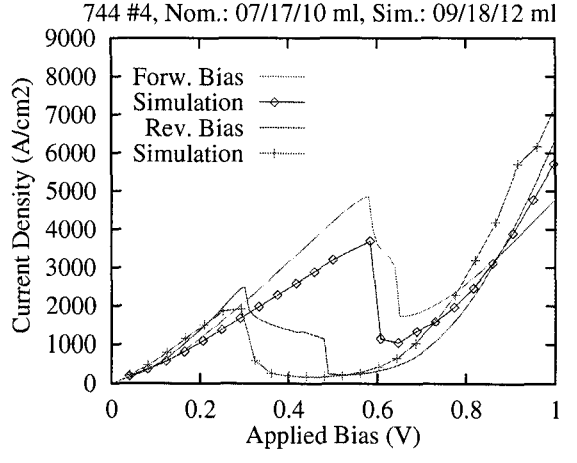

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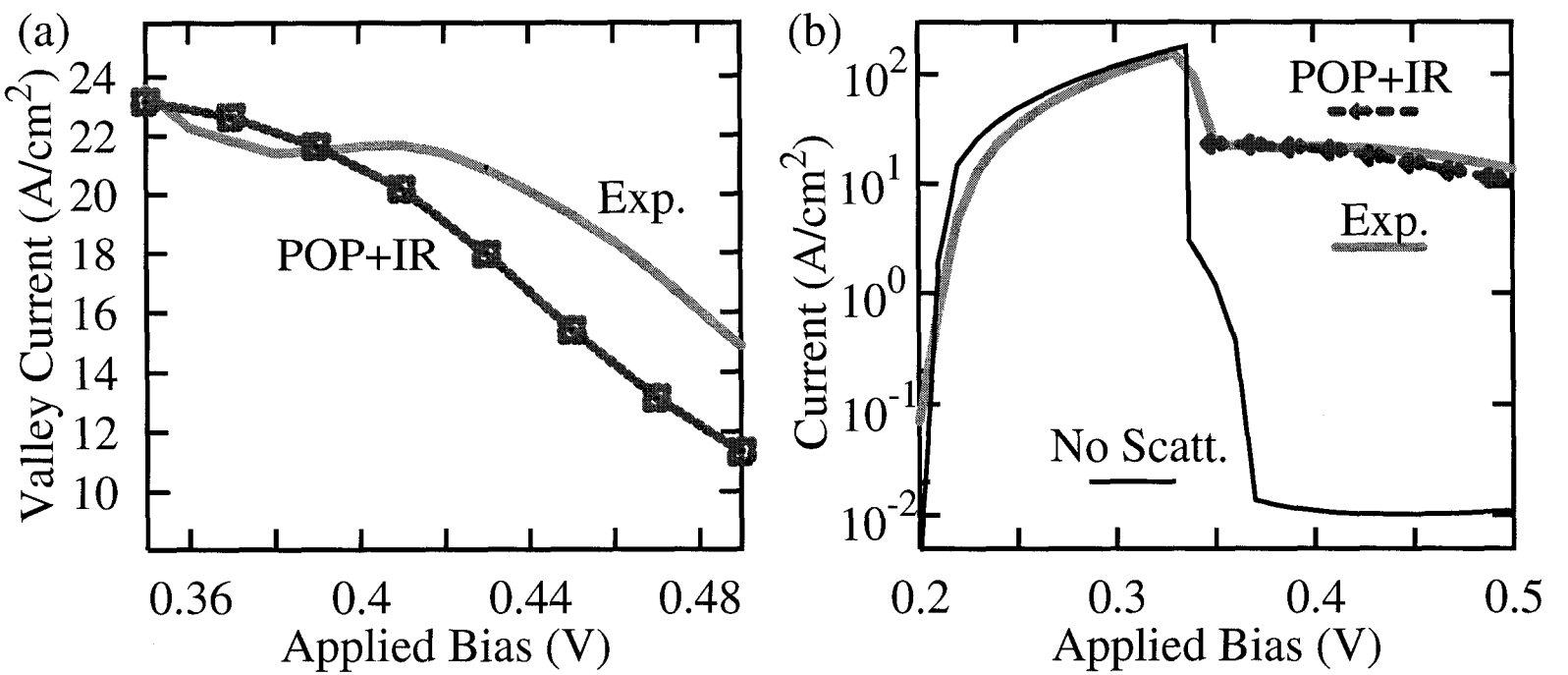

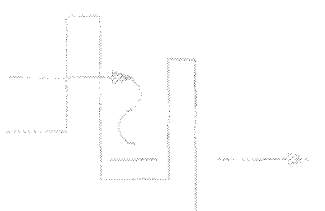

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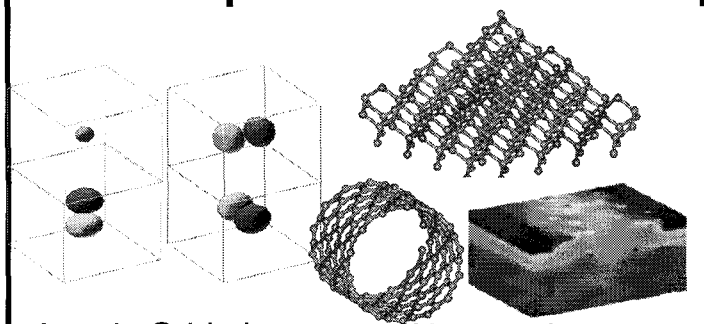

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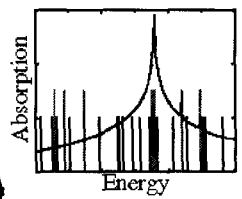

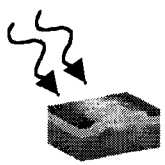

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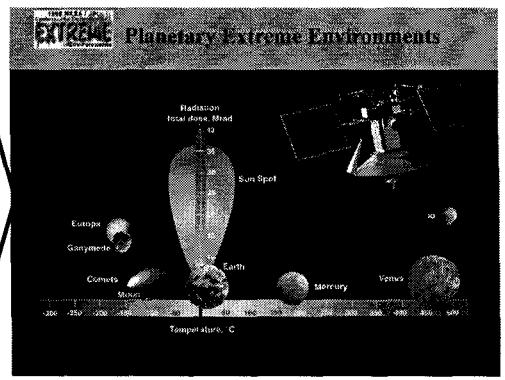

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Approach:

- Deliver a 3-D atomistic simulation tool
- Enable analysis of arbitrary crystal structures, particles, atom compositions and bond/structure at arbitrary temperatures and ambient electric and magnetic fields.

Collaborators:

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NASA Relevance:

- Enable new devices needed for NASA missions beyond existing industry roadmap:
  - Water detection -> 2-5μm Lasers and detectors.
  - Avionics -> High density, low power computing.
- Analyze state-of-the-art devices for non-commercial environments:
  - Europa -> Radiation and low temperature effects. Aging and failure modes.
  - Jovian system -> Magnetic field effects
  - Venus -> high temperature materials: SiGe

Impact:

- Low cost development of revolutionary techn.

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Modeling will narrow the empirical search space!

Speakers in the Program

- Carlo Jacoboni,
  Modena University,
  "The Wigner function and quantum transport"

- Harold Grubin,
  SRA, Inc.,
  "Modeling resonant tunneling diodes with Wigner functions and density matrices"

- Dejan Jovanovic,
  Motorola,
  "Non-equilibrium Green's functions for MOSFET modeling"

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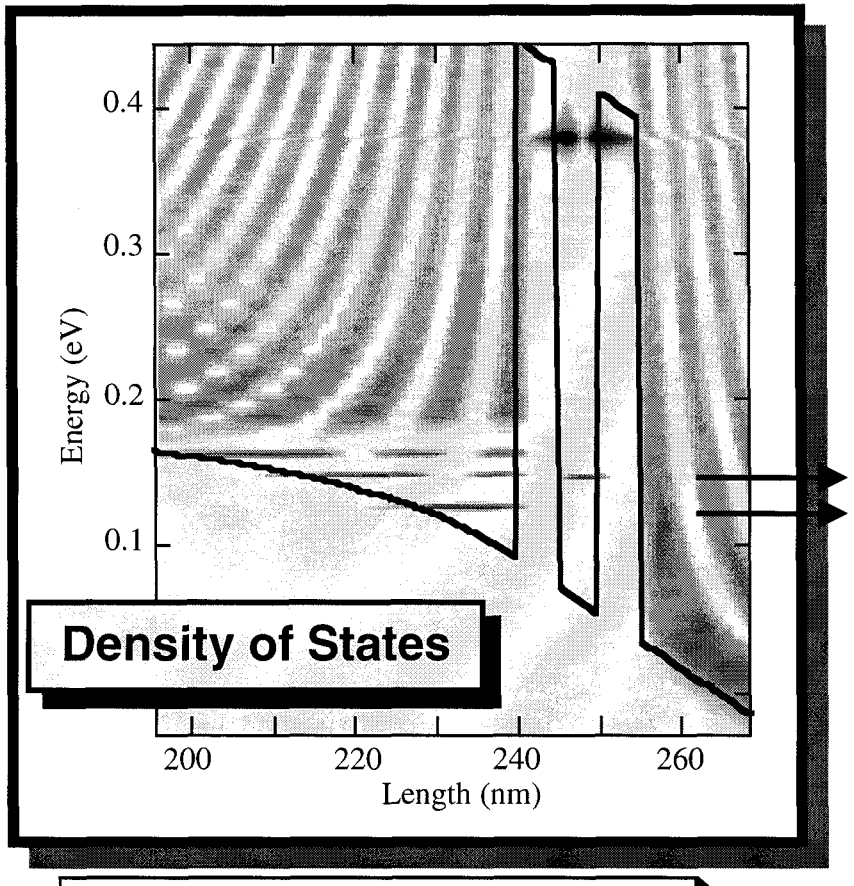

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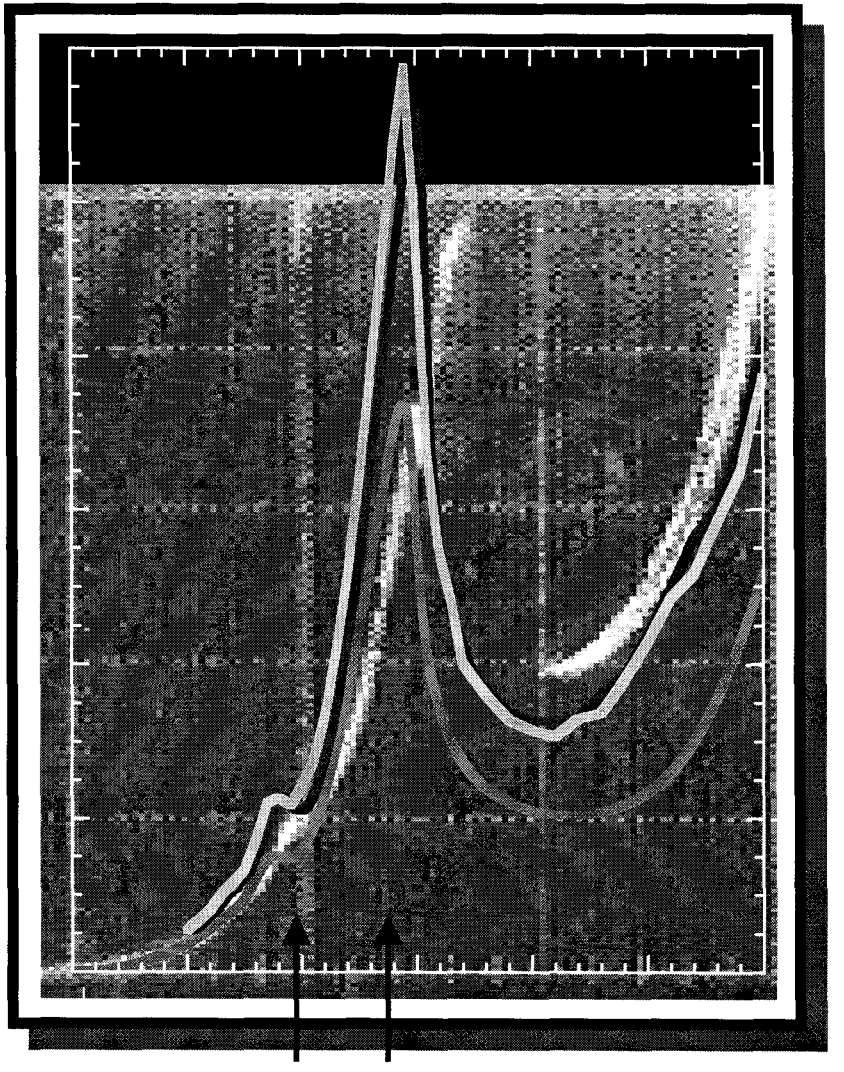

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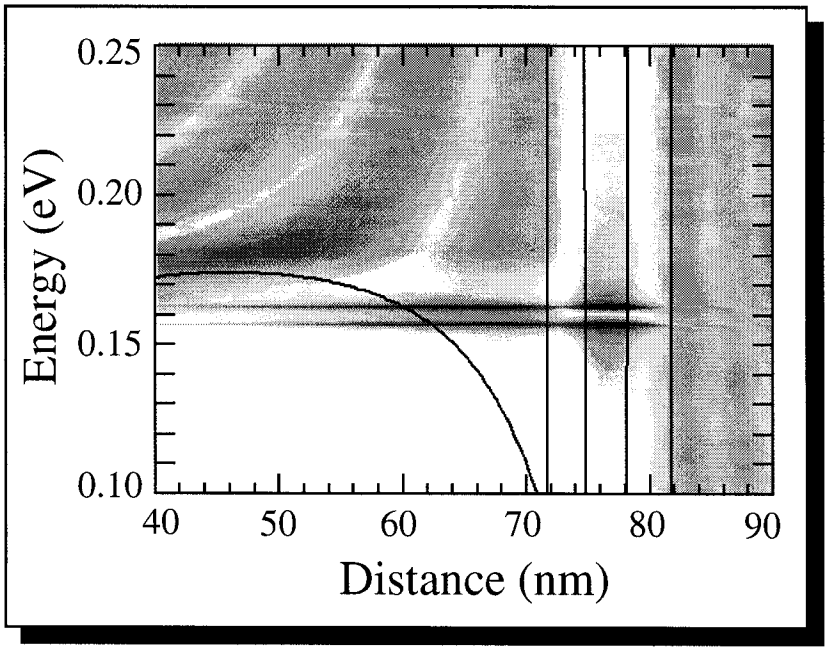

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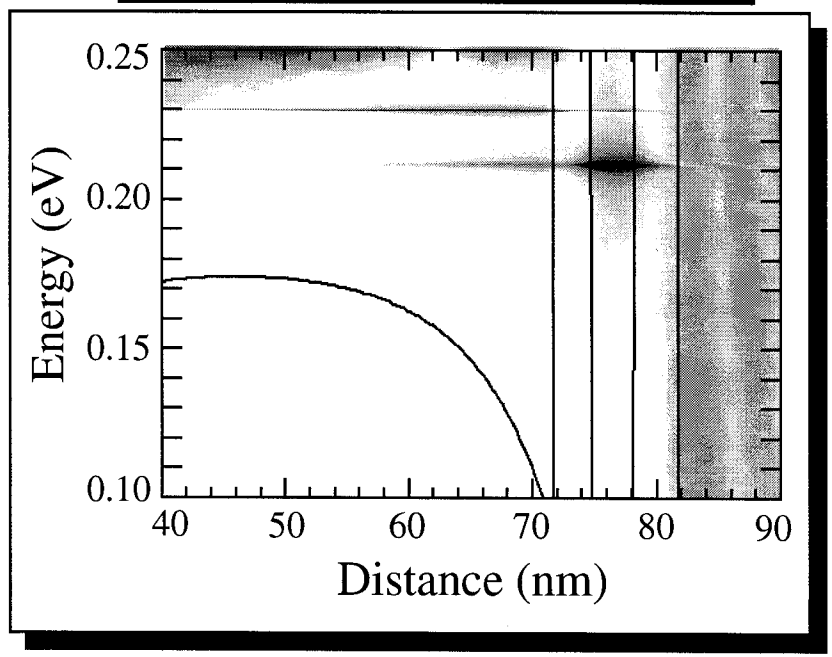

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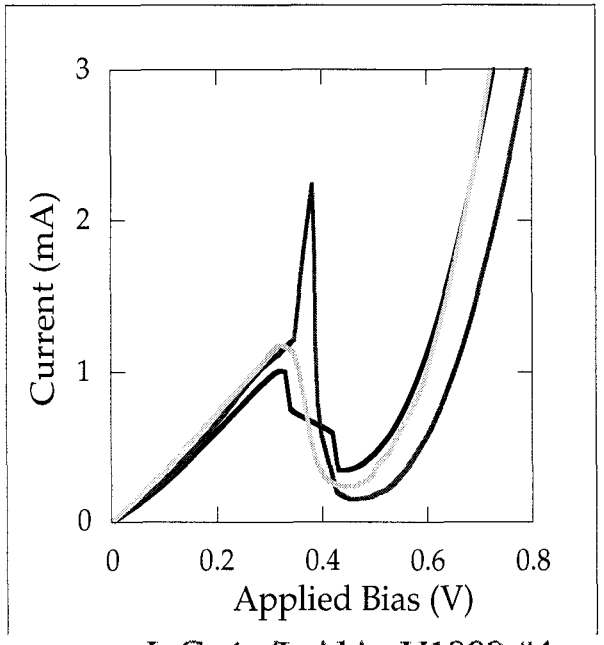

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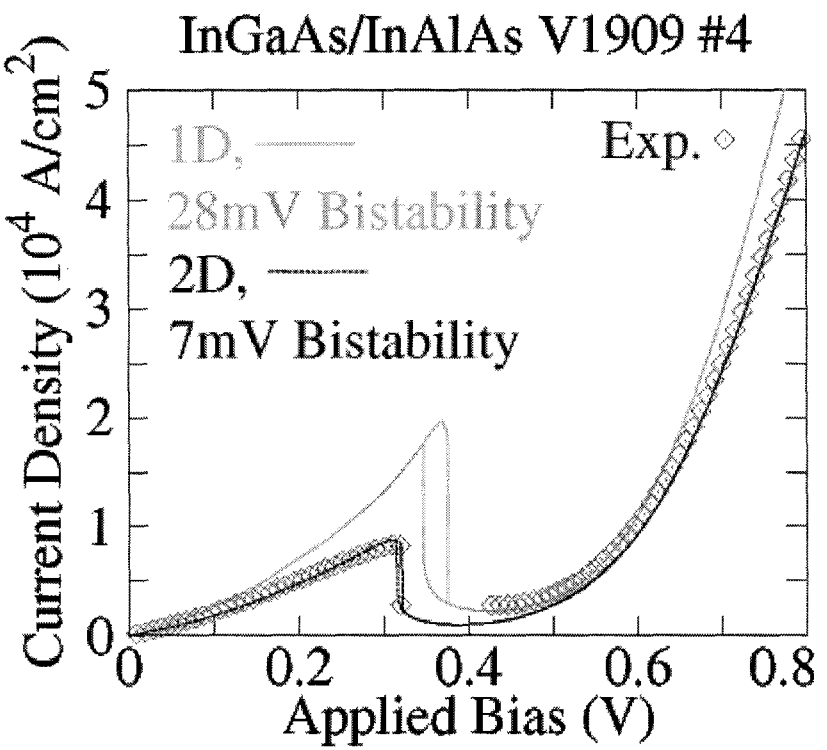

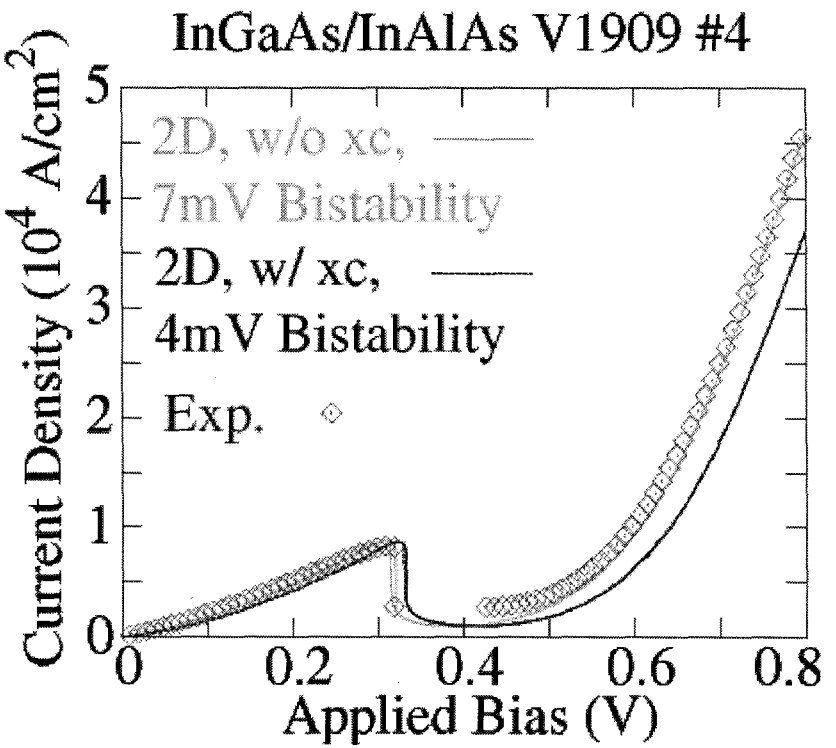

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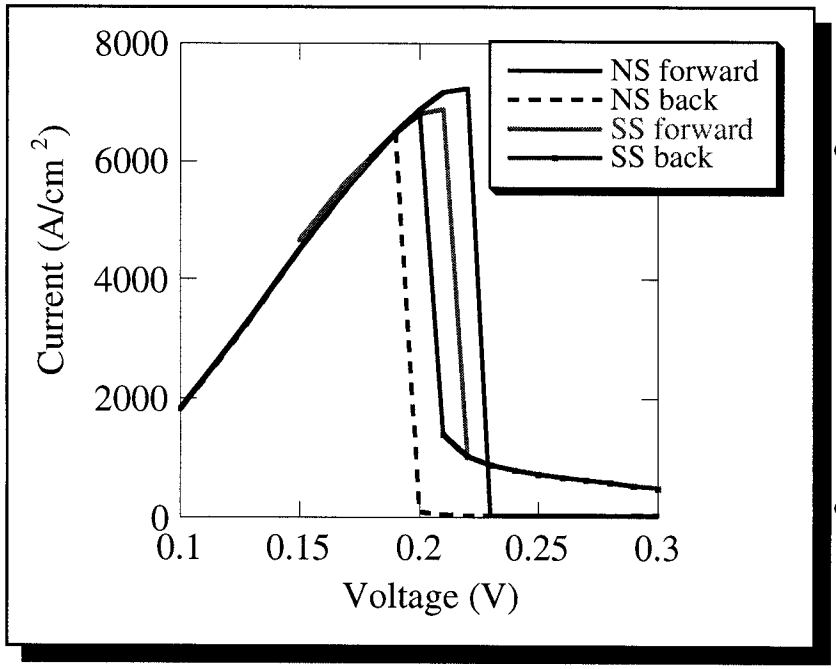

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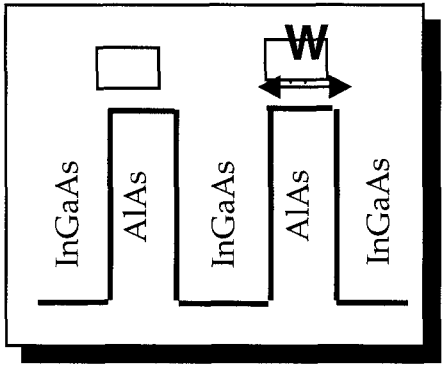

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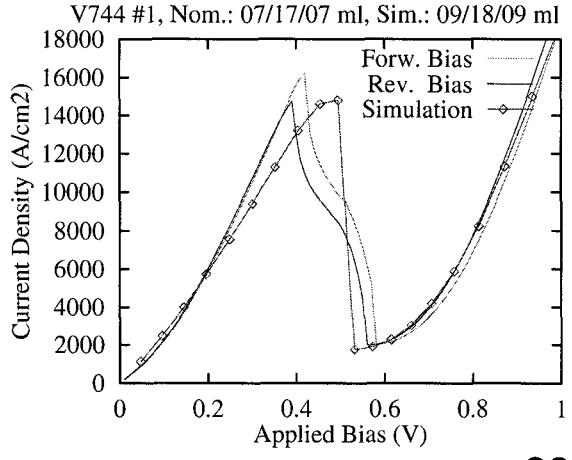

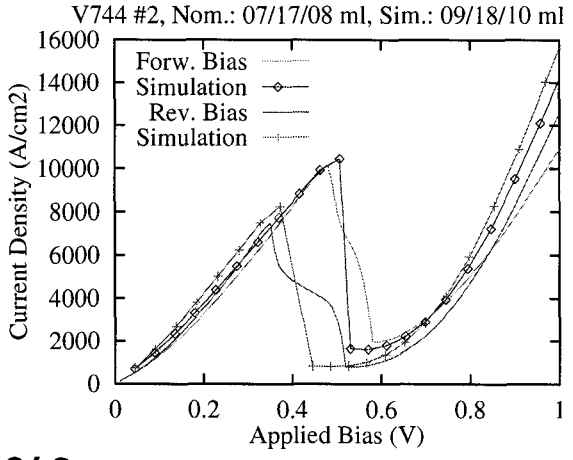

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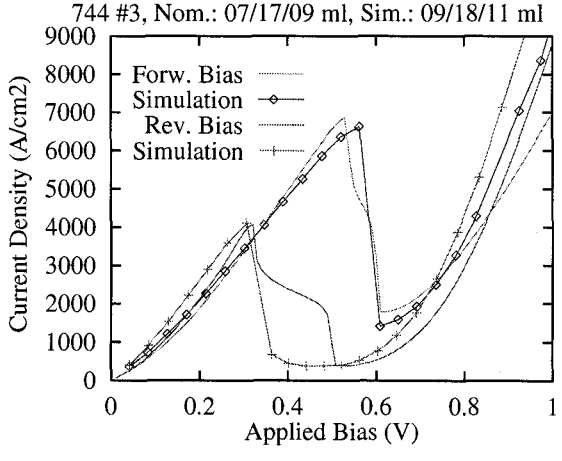

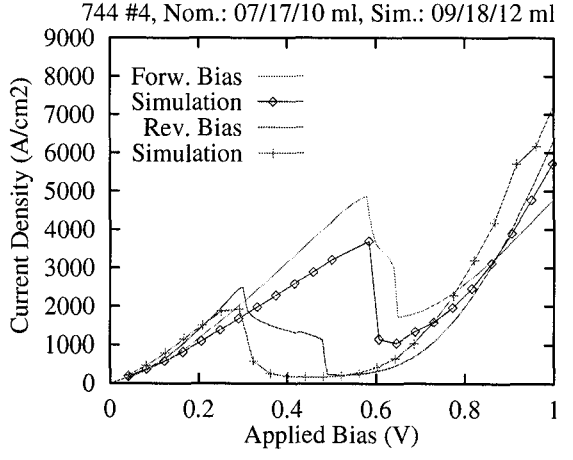

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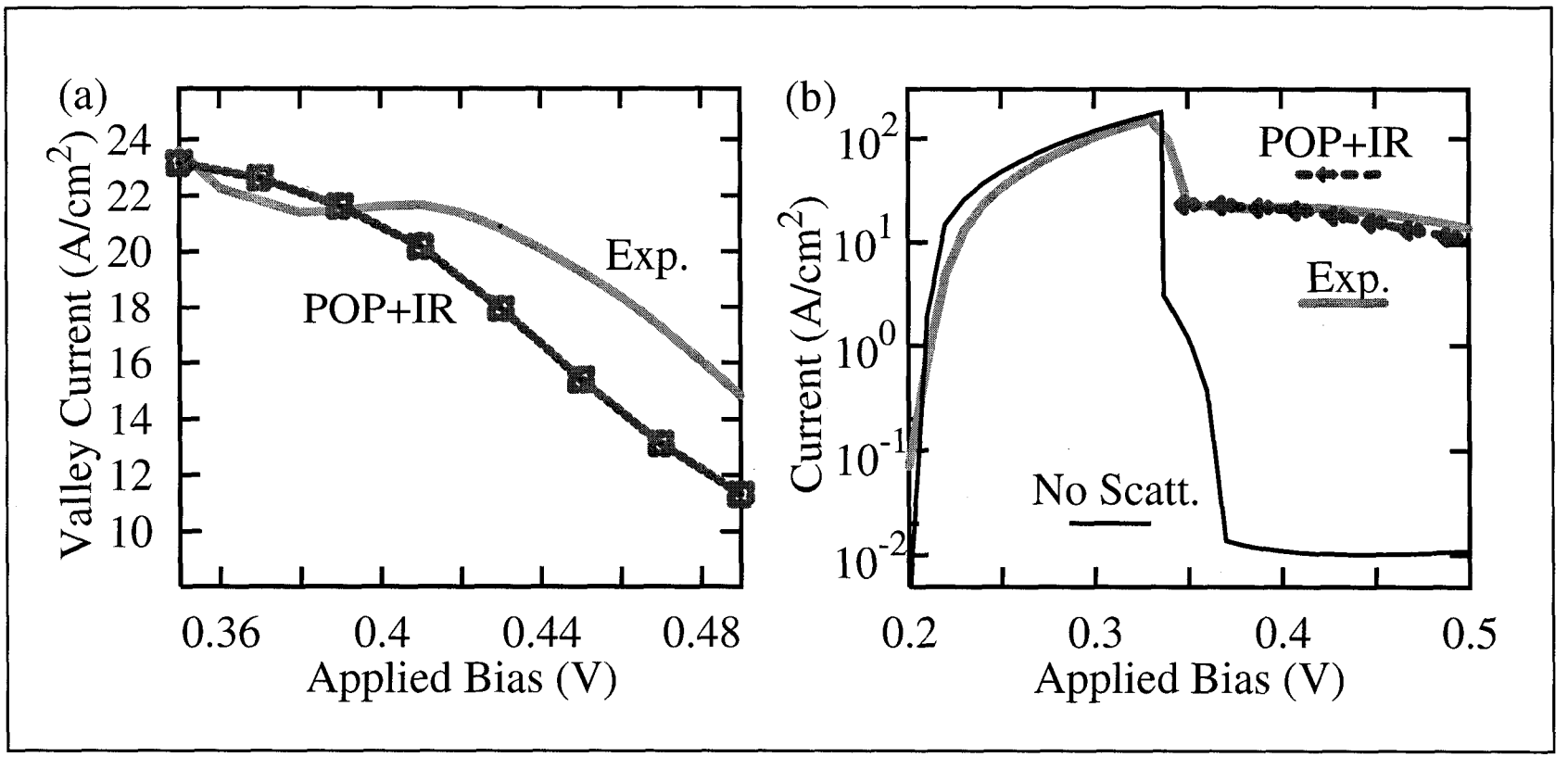

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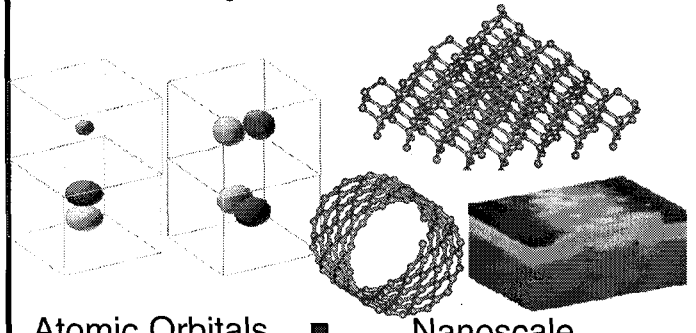

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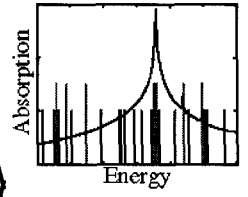

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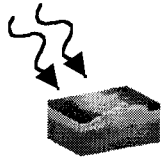

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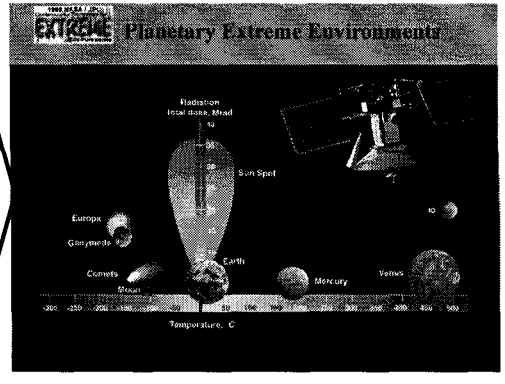

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- Enable new devices needed for NASA missions beyond existing industry roadmap:
  - Water detection -> 2-5μm Lasers and detectors.
  - Avionics -> High density, low power computing.
- Analyze state-of-the-art devices for non-commercial environments:
  - Europa -> Radiation and low temperature effects. Aging and failure modes.
  - Jovian system -> Magnetic field effects
  - Venus -> high temperature materials: SiGe

Impact:

- Low cost development of revolutionary techn.

Gerhard Klimeck

Modeling will narrow the empirical search space!

Speakers in the Program

- Carlo Jacoboni,
  Modena University,
  "The Wigner function and quantum transport"

- Harold Grubin,
  SRA, Inc.,
  "Modeling resonant tunneling diodes with Wigner functions and density matrices"

- Dejan Jovanovic,
  Motorola,
  "Non-equilibrium Green's functions for MOSFET modeling"